

Benzamide, N-(3-chlorophenyl)-2,3,4,5,6-pentafluoro-

Inchi:	InChI=1S/C13H5ClF5NO/c14-5-2-1-3-6(4-5)20-13(21)7-8(15)10(17)12(19)11(18)9(7)16/h
InchiKey:	GZUHDNOIYISDGC-UHFFFAOYSA-N
Formula:	C13H5ClF5NO
SMILES:	OC(=Nc1cccc(Cl)c1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	321.63

Physical Properties

Property code	Value	Unit	Source
hf	-983.50	kJ/mol	Joback Method
hvap	73.43	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.672		Crippen Method
mcvol	179.150	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	782.60	K	Joback Method
tc	988.33	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307377&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logP:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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